**Symposium A**

**P1-01** The coadsorption effect of Cl- and H2O on the various defect Al2O3 film surface  
Chuan-Hui Zhang, University of Science and Technology Beijing, China

**P1-02** Incorporation of double cross-slip in continuum dislocation dynamics  
Xingjia Zhou, Faculty of vehicle Engineering and Mechanics, Dalian University of Technology, China

**P1-03** Effect of defect on structural and optical properties in methyl-ammonium lead iodide (MAPI) perovskite via first principles calculations  
Abdullah Al Asad, Dept. of Electrical and Electronic Engineering, Okayama University, Japan

**P1-04** Isogeometric modeling and large-scale computation for stress field around lattice defects  
Shunsuke Kobayashi, Graduate School of Engineering, Osaka Univ., Japan

**P1-05** A local/nonlocal plasticity model for upscaling microstructural effects  
John Mitchell, Sandia National Laboratories, United States of America

**P1-06** First-principles investigation of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface  
Zhong-min Wang, Guilin University of Electronic Technology, China

**P1-07** First-principles study on electronic properties of hybrid MABX3 perovskites (MA= CH3NH3+, B= Pb, Sn, Ge; X= I, Br, Cl)  
Narasak Pandech, School of Physics and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials, Suranaree University of Technology, Thailand

**Symposium C**

**P1-08** Pressure effects on dislocation core structures in Mg2SiO4 olivine: insights from atomic-scale modeling  
Philippe Carrez, Lille University, Lab. UMET UMR-CNRS 8207, France

**P1-09** Structural and magnetic properties of long-period stacking ordered (LPSO) structure of iron; a first-principles study  
Takao Tsumuraya, Magnesium Research Center/POIE, Kumamoto Univ., Japan

**P1-11** Dislocation transmission behaviors of bi-crystal BCC tantalum with high and low angle symmetric tilt grain boundaries: multiscale simulation study  
Moon Sunil, Dept. of Mechanical Engineering, Yonsei Univ., Korea

**P1-12** Ab Initio dislocation core calculations using a cluster model  
Jonas Frafjord, Dept. of Physics, Norwegian University of Science and Technology, Norway

**P1-13** Anelastic recovery of a steel wire under pure shear strain with various magnetic treatments  
Shigeo Kotake, Dept. of Mechanical Engineering, Mie Univ., Japan

**Symposium E**

**P1-14** Possible explanation of sudden stress drop at upper yield point in iron by magnetostriction and unpinning dislocations with law of approach in residual magnetization  
Shigeo Kotake, Dept. of Mechanical Engineering, Mie Univ., Japan

**P1-15** Investigation of dislocation core structure in aluminum by using a generalized Peierls-Nabarro model  
Hideki Mori, College of Industrial Technology, Japan

**P1-16** Crystal orientation evolution analysis during deformation using molecular dynamics  
Keisuke Kinoshita, Nippon Steel & Sumitomo Metal Corporation, Japan

**P1-17** Nanoindentation of nanoparticles – a molecular dynamics and discrete dislocation dynamics simulations study  
Dan Mordehai, Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel

**P1-18** Machine learning interatomic potentials for molecular dynamics simulations of dislocations  
Eyal Oren, Dept. of Materials Engineering, Ben-Gurion University of the Negev, Israel

**P1-21** Large-scale molecular dynamics simulations: coupling with dislocation dynamics  
Pavel A. Pokatashkin, Dukhov Research Institute of Automation (VNIIA), Russia

**P1-22** Hydrogen embrittlement controlled by reaction of dislocation with grain boundary in alpha-iron polycrystals  
Liang Wan, Wuhan University, China

**P1-23** Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed kinetic Monte Carlo method  
Shuhei Shinzato, Dept. of Mechanical Science and Bioengineering, Osaka Univ., Japan

**P1-24** Molecular dynamics simulations of low-cycle fatigue behavior in single layer molybdenum disulfide  
Yu-Cheng Su, National Chiao Tung University, Taiwan

**P1-25** Fracture behavior of multi-walled carbon nanotube under biaxial loading condition  
Masamichi Nishimura, Dept. of Mechanical Systems Engineering, Shinshu Univ., Japan

**P1-26** On the role of amorphous shells on mechanical properties of fcc Ni nanoparticles under compression  
Alexandra Goryaeva, DEN-Service de Recherches de Metallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

**P1-27** Molecular dynamics analysis of hydrogen diffusion behavior in alpha-Fe bi-crystal under stress gradient  
Ken-ichi Saitoh, Kansai Univ., Japan

**P1-28** Understanding interactions of dislocations with interfaces in nickel-based superalloys: insights from molecular dynamics simulations  
Jian Huang, Shanghai Institute of Ceramics Chinese Academy of Sciences, China
P1-29 The influence of nano-sized Ti3Al particles on the mechanical properties of α-titanium alloys
Yan He, IMR, CAS, China

P1-30 The atomic study of tensile property for nickel nanowires with helium bubble
Hengfeng Gong, CGN, China

P1-31 Components of fracture response of alkali-activated slag mortars with steel fibers
Hana Simonova, Brno University of Technology, Faculty of Civil Engineering, Czech Republic

P1-32 Molecular dynamics simulation of crack growth behavior of single crystal γ-TiAl alloy under different Nb substitution mode
Yuxi Feng, Mechanical and Electronical Engineering College, Lanzhou University of Technology, China

P1-33 Understanding of delayed hydride cracking failure mechanism in E110 zirconium based fuel claddings by EBSD and in-situ mechanical testing
Hygreaa Kiran Namburi, Research Centre REZ, Czech Republic

P1-34 Transition-metal alloying of γ′-Ni3Al: effects on the ideal uniaxial compressive strength from first-principles calculations
Minru Wen, Tsinghua University, China

P1-35 The influence of deposition pattern on stress and mechanical properties in wire arc additive manufacturing
Changmeng Liu, Beijing Institute of Technology, China

P1-36 On the significance of the higher-order neighbors for abnormal grain growth and recrystallization nucleation
Markus Kuehbach, Max-Planck-Institut fuer Eisenforschung GmbH, Germany

P1-37 Hydrogen trapping in carbon supersaturated a-iron and its decohesion effect in martensitic steel
Wen-Tong Geng, Department of Mechanical Science and Bioengineering, Osaka University, Japan

P1-38 Size scale effect on energy absorption property of aluminum foam
Zengyou Liang, North University of China, China

P1-39 Development of charge-transfer type interatomic potential for SiC oxidation
So Takamoto, The Univ. of Tokyo, Japan

P1-40 Alpha-phase in engineering aluminum alloys: a multiscale modeling approach to its mechanical behavior
Duancheng Ma, Leichtmetallikompetenzzentrum Ranshofen GmbH, Austria

P1-41 Multi-phase-field lattice Boltzmann modeling and simulation of equiaxed structure
Ryotaro Sato, Kyoto Institute of Technology, Japan

P1-42 Simulation of extrusion process of TiAl alloy prepared by triple VAR
Fan Gao, AECC Beijing Institute of Aeronautical Materials, China

P1-43 Experimental-computational analysis of primary static recrystallization in DC04 steel
Martin Diehl, Max-Planck-Institut fuer Eisenforschung GmbH, Germany

P1-44 Combining 4D experiments and phase-field modeling to determine reduced grain boundary mobilities
Jin Zhang, Northwestern University, United States of America

P1-45 Fiber-intersectant microstructure of fish scale and biomimetic research
Bin Chen, College of Aerospace Engineering, Chongqing University, China

P1-46 Microstructures of turtle shell and biomimetic fabrication
Bin Chen, College of Aerospace Engineering, Chongqing University, China

P1-47 Phase-field simulation of solidification process in welding pool of Fe-C binary alloy
Lan Zhan, Jiamusi Univ., China

P1-48 Phase field simulation of the phase separation in the TiC-ZrC-WC system
Zein Luq, State Key Lab of Powder Metallurgy, Central South University, China

P1-49 Switching of coordinate transformations of a repetitive bar-and-joint framework under uniaxial compression
Hiro Tanaka, Dept. of Mechanical Engineering, Osaka Univ., Japan

P1-50 Understanding the effect of residual stresses in 3D printed metals
Alankar Alankar, IIT Bombay, India

Symposium F

P1-33 Understanding of delayed hydride cracking failure mechanism in E110 zirconium based fuel claddings by EBSD and in-situ mechanical testing
Hygreaa Kiran Namburi, Research Centre REZ, Czech Republic

P1-34 Transition-metal alloying of γ′-Ni3Al: effects on the ideal uniaxial compressive strength from first-principles calculations
Minru Wen, Tsinghua University, China

P1-35 The influence of deposition pattern on stress and mechanical properties in wire arc additive manufacturing
Changmeng Liu, Beijing Institute of Technology, China

Symposium H

P1-51 Multi-scale modeling of DNA-dendrimers in electrolyte solutions
Natasa Adzic, Faculty of Physics, University of Vienna, Austria

P1-52 Structural and dynamical properties of star block-copolymers in shear flow
Diego Felipe Jaramillo-Cano, Faculty of Physics, University of Vienna, Austria

P1-53 Multiscale simulation of polymeric solids for fracture processes
Takahiro Murashima, Dept. of Physics, Tohoku Univ., Japan

P1-54 Quantification and validation of the mechanical properties of DNA nicks
Jae Young Lee, Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea

P1-55 Investigating the mechanical properties of azobenzene-tethered DNA for controlling self-assembling DNA nanostructures
Jae Gyung Lee, Dept. of Mechanical and Aerospace Engineering, Seoul National Univ., Korea

P1-56 FTMP-based modeling and simulations of glassy polymers
Soushi Miyamoto, Dept. of Mechanical Engineering, Kobe Univ., Japan

P1-57 Shock wave induced damage in tumor cells: experiments and simulations
Martin Steinhauser, Fraunhofer Ernst-Mach-Institute, EMI, Germany
Symposium I

P1-58 Phase-field modeling of anisotropic grain growth with incorporation of Sigma 3 CSL grain boundaries
Kunok Chang, Kyung Hee Univ., Korea

P1-59 Direct mapping from molecular dynamics to phase-field simulations for accurate prediction of grain growth
Eisuke Miyoshi, Kyoto Institute of Technology, Japan

P1-60 Density functional theory plus Hubbard U study of the segregation of Pt to the CeO$_2$ grain boundary
Zhixue Tian, Hebei Normal Univ., China

P1-61 Interfacial charge transfer and enhanced photocatalytic mechanism for Bi$_2$WO$_6$/BiOCl heterostructure: a first-principles theoretical study
Pan Li, Hebei Normal Univ., China

P1-62 Investigation of abnormal grain growth conditions by phase-field method
Nobuko Mori, Kyoto Institute of Technology, Japan

P1-63 Phase field crystal modeling of mechanism of strain-driven for nucleation and grain of deformed-grain
Ying-Jun Gao, Guangxi University, China

P1-64 Diffusion and trapping of hydrogen at grain boundaries scale in fcc polycrystalline nickel: some implications of theatomic volume and the interstitial self-stress
Xavier Feaugas, University of La Rochelle, France

Symposium J

P1-65 Multiscale model for interlayer defects in heterogeneous bilayer material
Shuyang Dai, Wuhan University, China

Symposium L

P1-66 Molecular dynamics study on temperature and loading rate dependence of nano-indentation pop-in load
Yuii Sato, Department of Mechanical Science and Bioengineering, Osaka University, Japan

P1-67 Geometry of curved surface and energetics of in graphene with defects
Ako Kihara, Dept. of Mechanical Engineering, Univ.of Fukui, Japan

P1-68 Collective motion of dislocation associated with local plasticity initiation and subsequent behavior in bcc metals
Takahito Ohmura, National Institute for Materials Science, Japan

Symposium M

P1-69 Formation of physical gels by arrested spinodal decomposition in charged colloids
Jose Manuel Olais-Govea, Instituto Tecnologico y de Estudios Superiores de Monterrey, Mexico

P1-70 How to improve the ductility of CuZr BMGs based on cyclic pre-straining: MD simulations and mechanical testing
Jonathan Amodeo, MATEIS, Univ. Lyon 1, France

P1-71 Modeling plastic deformation of amorphous solids from atomic scale mechanisms
Francesca Boioli, LEM, CNRS-ONERA, Chatillon, France

P1-72 Thermally activated creep and constant shear rate deformation in amorphous materials
Samy Merabia, CNRS and Universite Lyon 1, France

P1-73 Numerical analysis of shrinkage process based on the experimental data
Barbara Kucharczykova, Brno University of Technology, Faculty of Civil Engineering, Institute of Building Testing, Czech Republic

Symposium O

P1-74 Designing lubricant additives for titanium carbide surface: first-principles and molecular dynamics investigations
Tasuku Onodera, Research & Development Group, Hitachi, Ltd., Japan

P1-75 Crystal growth molecular dynamics simulation of alpha-Al$_2$O$_3$ cutting tools for realizing their best tribological properties
Shandan Bai, KYOCERA Cop., Japan

P1-76 Atomistic modeling of polymer friction
Robin Sam Vacher, SINTEF-NTNU, Norway

P1-77 A two degree-of-freedom extension to the Prandtl Tomlinson-model for friction strengthening in layered materials
David Andersson, Department of Physics, Stockholm University, Sweden

P1-78 Analysis of friction characteristics of steel powders using parallelized discrete element method
Naoki Yashiro, Graduate School of Simulation Studies, University of Hyogo, Japan

P1-80 Dynamics of polymer under shear in confinement geometry
Taiki Kawate, Univ. of Hyogo, Japan

P1-81 Dynamics of a polymer in bulk solution under shear flow
Soma Usui, Univ. of Hyogo, Japan

P1-82 Mechanochemistry induced atomic wear in chemical mechanical polishing processes
Jialin Wen, Dept. of Mechanical Engineering, Tsinghua Univ., China

P1-83 Adsorption property of a fatty acid on iron surface with grain boundary
Yuki Uchiyama, Toyota Technological Institute, Japan
Symposium A

P2-01 Multiscale model of solid state amorphization during processing of pharmaceutical materials
Alejandro Strachan, Purdue University, United States of America

P2-02 FTMP-based modeling and simulations of HCP Mg single crystal
Takahiro Kitano, Dept. of Mechanical Engineering, Kobe Univ., Japan

P2-03 Nonlinear elasticity on Riemannian manifold and its application to general surface development
Yuto Horikawa, Dept. of Mechanical Engineering, Osaka Univ., Japan

P2-04 The challenge of achieving quantitative phase field models for microstructure evolution in irradiated solids - the case of voids
Anter El-Azab, Purdue University, United States of America

P2-05 A molecular-dynamics study of surface tension: from alloy droplets to bubbles in molten alloy
Xiangming Ma, East China Normal University, China

Symposium B

P2-06 Effects of rhenium on the mechanical behavior of irradiated tungsten: a molecular dynamics study using neural-network potential
Ryo Kobayashi, Nagoya Institute of Technology (NITech), Japan

P2-07 Diffusion behavior and temperature dependence of hydrogen in tungsten and molybdenum under isotropic strain state
QuanFu Han, Beihang University, China

P2-08 Diffusion of point defects on tungsten surface
Shuo Jin, School of Physics and Nuclear Energy Engineering, Beihang University, China

P2-09 Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten
Ying Zhang, Beihang University, China

P2-10 Screw dislocation-interstitial solute coevolution in W-O alloys using atomistically-informed kinetic Monte Carlo simulations
Yue Zhao, Dept. of Materials Science and Engineering, University of California, Los Angeles, United States of America

P2-11 Kinetic Monte-Carlo simulations of radiation damage in W(Re,Os) alloys
Matthew James Lloyd, Department of Materials, University of Oxford, UK

P2-12 Dynamics of magnetism in neutron irradiated iron-chromium steels
Jacob B. J. Chapman, Culham Centre for Fusion Energy (CCFE), UK

Symposium C

P2-14 Atomistic insights into the grain boundaries interaction with radiation-induced point defects in bcc Fe-Cr alloys
Marcin Roland Zemla, Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland

P2-15 Production and process of cascade development in irradiated pure α-Zr from molecular dynamics simulations
Rongqian Pan, The First Sub-Institute, Nuclear Power Institute of China, China

P2-16 Microstructure evolution of cascade annealing in irradiated pure α-Zr from molecular dynamics simulations
Bang Wei, The First Sub-Institute, Nuclear Power Institute of China, China

P2-18 Prediction of biaxial tensile deformation behavior of aluminum alloy sheets using crystal plasticity finite element method and machine learning
Kota Koenuma, Tokyo University of Agriculture and Technology, Japan

P2-19 MobiDIC: a 3-D dislocation dynamics simulation
Ronan Madec, CEA, DAM, DIF, France

P2-20 Temperature dependence of fatigue crack growth in Ti6Al-4V
Bhargavi Rani Anne, Dept. of Materials Science and Engineering, Kyushu University, Japan

P2-21 Parametric model of discrete dislocation dynamics based on mathematical theory of moving curves
Miroslav Kolar, Czech Technical University in Prague, Czech Republic

P2-22 On visualization of multiscale information transfer/exchange processes via FTMP-based duality diagram representation scheme
Takuya Takaai, Dept. of Mechanical Engineering, Kobe Univ., Japan

P2-23 Rotational field evolutions based on field theory of multiscale plasticity (FTMP)
Tadashi Hasebe, Kobe Univ., Japan

P2-24 A 2D mesoscale study of dislocations, cracks and martensitic phase transformations
Rachel Derby, TU Bergakademie Freiberg, Germany

P2-25 Effects of stress distribution on the plastic deformation of metallic glasses under different geometries
Chih-Jen Yeh, National Cheng Kung University(Taiwan), 2.Chung Yuan Christian University, Taiwan

Symposium D

P2-26 Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles
Abhijit Chatterjee, Dept. of Chemical Engg., Indian Institute of Technology Bombay, India

P2-27 Development of thermodynamic database of Nd-Fe-B-based permanent magnet alloys
Jiang Wang, School of Material Science and Engineering, Guilin University of Electronic Technology, China
**Symposium E**

**P2-34** Design of proteins and biopolymers: role of directional interactions and of water.  
Valentino Biondo, University of Vienna, Austria

**P2-28** Design of spontaneous formation- based 3D plasmonic optical structure, using multypehysics modeling  
Jihwan Song, Dept. of Mechanical Engineering, Hanbat National University, Korea

**P2-35** Optimization of elastic moduli of the silicate glasses through high-throughput atomistic modeling and machine learning techniques  
Liang Qi, Dept. of Materials Science and Engineering, University of Michigan, United States of America

**P2-44** Characterization of KxNa1-xNbO3 powders and ceramics prepared by hydrothermal synthesis  
Jing Yang, Dept. of Materials Science and Engineering, Xi An Univ. of Science and Technology, China

**P2-36** High pressure phase transition and structural stability of transition metal compounds  
Fanyan Meng, Dept. of Physics, University of Science and Technology Beijing, China

**P2-45** Numerical and experimental investigation of liquid metal dealloying of Cu-Ni alloy in liquid silver.  
Pierre-Antoine Geslin, INSA Lyon/CNRS, France

**P2-37** Development of artificial neural network model for prediction of electronic density of states in atomistic systems  
Atsushi Kubo, Institute of Industrial Science, the University of Tokyo, Japan

**P2-46** Application of DLVO theory to predict dispersion stability of ZrO2 submicron particles in electrolyte solutions  
Ming-Hong Chueh, Industrial Technology Research Institute, Taiwan

**P2-38** Development of first-principles platform technology for energy research  
Kanghoon Yim, R&D Platform Center, Korea Institute of Energy Research, Korea

**P2-47** Multi-GPU large-scale phase-field lattice Boltzmann simulation of dendrite growth with thermal-solutal convection  
Shinji Sakane, Kyoto Institute of Technology, Japan

**Symposium F**

**P2-39** Dynamics of a solidification front made by invasion of fluid with a different temperature  
So Kitsunezaki, Nara Women's Univ., Japan

**P2-50** Molecular-dynamic simulation of rapid solidification of dipolar molecular crystal from its melt  
Xiang Xu, East China Normal University, China

**P2-40** Strengthening through solid solution in W1-xTaxB system  
Lijuan Liu, Dept. of Applied Physics, University of Science and Technology Beijing, China

**P2-51** Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation  
Shih Kuang Lee, National Chiao Tung University, Taiwan

**P2-37** Desiccation crack patterns based on phase-field modeling and their statistical properties  
Shin-ichi Ito, The Univ. of Tokyo, Japan

**P2-52** Intrinsic analysis of structural order parameter at equilibrium crystal-melt interfaces  
Wenliang Lu, East China Normal University, China

**P2-41** Comparison of different alkali activated mortars with hemp fibres response during fracture test by acoustic emission method  
Hana Simonova, Brno University of Technology, Faculty of Civil Engineering, Czech Republic

**P2-53** Multiscale modelling of indirect-to-direct band gap transition in silicon nanosheets  
Byung-Hyun Kim, R&D Platform Center, Korea Institute of Energy Research, Korea

**Symposium G**

**P2-39** Numerical analysis of elasto-plastic behavior of metallic architected materials  
Filip Siska, Institute of Physics of Materials, Czech Academy of Sciences, Czech Republic

**P2-54** Component-wise effect of incompatibility tensor on misorientation development in lath block structure model based on FTMP  
Yuta Amano, Dept. of Mechanical Engineering, Kobe Univ., Japan

**P2-40** Automatic analysis and numerical prediction of flow stress curves for aluminium alloys  
Evgeniya Kabilman, Light Metals Technologies Ranshoven, Center fo Low-Emission Transport, Austrian Institute of Technology, Austria

**P2-55** Construction of virtual ITZ specimens using extended stochastic optimization and evaluation of their permeability  
Se-Yun Kim, Dept. of Civil and Environmental Engineering, Yonsei Univ., Korea
Symposium H

P2-58 Studying the kinetics of a self-propelled cruiser in 2D granular media under gravity
Guc-lle Jason Gao, Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan

P2-59 A discrete tetris model showing two flow regimes for hard particles exiting a hopper with an adjustable obstacle
Tomoya Yasuno, Dept. of Mathematical and Systems Engineering, Shizuoka Univ., Japan

P2-60 Effect of water molecules on polymer chain motion in dense chain ensembles of nanofiber membrane
Isamu Riku, Osaka Prefecture Univ., Japan

P2-61 A coarse-grained model for competitive adsorption on the surface of inorganic nanomaterials
Stefano Poggio, School of Physics, University College Dublin, Ireland

P2-62 Molecular dynamics of inorganic and organic interfaces with force-field parameters based on DFT simulations
Kosuke Ohata, JSOL Corporation, Japan

P2-63 Molecular dynamics screening for developing compounds of electrolytes with high performance in lithium ion batteries
Yoshihiro Takai, Graduate school of Science and Engineering, Kansai Univ., Japan

P2-64 Molecular dynamics study on transmission mechanism of torsional deformation in cellulose nanofibers with hierarchical structure
Kentaro Takada, Graduate School of Science and Engineering, Kansai Univ., Japan

P2-65 Bubble dynamics of foam flow around an obstacle
Antti Puisto, Aalto University, Department of Applied Physics, Finland

P2-66 Shape deformation and mechanical relationship of ionic droplet under an electric field
Wei-Chun Lin, Department of Civil Engineering, National Cheng Kung University, Taiwan

P2-67 Multiscale modeling of surface functionalized graphene/polymer nanocomposites: insight into the effect of covalent grafting
Jeong-ha Lee, Dept. of Energy Engineering, Chung-Ang Univ., Korea

P2-68 Durability analysis on the environmental aging of epoxy-based nanocomposite
Sunyong Kwon, Dept. of Energy Engineering, Chung-Ang Univ., Korea

Symposium I

P2-69 Topological evolution of the microstructures of thin films during grain growth
Abu Oencue, Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany

P2-70 Molecular dynamics simulations of phase transformations in nanocrystalline NiTi shape-memory alloys
Won-Seok Ko, University of Ulsan, Korea

P2-71 An attempt to connect migration of grain boundaries to their atomic structures with help of molecular dynamics
Sylvain Queyreaux, Universite Paris XIII, France

P2-72 Disconnection interaction in Cu grain boundaries
Christian Brandl, Karlsruhe Institute of Technology, Germany

P2-73 Phase-field approach to thermo-mechanical behavior of through-silicon vias
Jaekeun Yoon, Sogang Univ., Korea

P2-74 Grain-growth in nanocrystalline metals under ion irradiation: a thermal spike model
Djamel Kaoumi, North Carolina State University, United States of America

Symposium N

P2-75 Why the structure-property relationship in metallic glasses should be established beyond short-range order: insight from potential energy landscape
Dan Wei, University of Chinese Academy of Sciences, China

P2-76 Vacancy segregation analysis near grain boundaries in metallic systems by long-time atomistic simulations
Shotaro Hara, Dept. of Mechanical Engineering, Chiba Institute of Technology, Japan

P2-77 Experimental and density functional theory studies of precipitate interfaces in aluminium alloys, with focus on $\beta^\prime$ & $\beta$
Haris Rudianto, Gunadarma University, Indonesia

Symposium O

P2-78 Adsorption of volatile organic compounds (VOCs) on silicene by density functional theory calculations
Thi Viet Bac Phung, Nanotechnology Program, Vietnam National University – Vietnam National University, Viet Nam

P2-79 Atomistic insights into defect formation mechanism in single crystal SiC based on molecular dynamics simulation
Kenji Nishimura, AIST, Japan

P2-80 Potential cathode material Na$_2$VOPO$_4$ for rechargeable sodium – ion batteries: DFT investigation
Duc Huu Luong, Nano Technology Program, Vietnam University, Viet Nam

P2-81 Two-dimensional Na$_2$SiS as a promising anode material for rechargeable Sodium-based batteries: ab initio material design.
Van An Dinh, Nanotechnology Program, Vietnam National University, Viet Nam

P2-82 Modelling and analysis of SiO$_2$ interfaces of non-firing solids
Tomohiro Sato, Dept. of Mechanical Engineering, Kansai Univ., Japan